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J2142-1

Graph-Set Analysis of Individual Structures

The following is a discussion of the intermolecular interactions in salts **1-6** in terms of graph sets. The analysis here is limited to first- and second-level graph sets. Related structures are compared in terms of graph sets in the published manuscript.

DL-Lysine/HABS (1). With one exception, the first-level hydrogen-bonding motifs found in **1** are finite interactions of the **D** type (Table Supp-1). The exceptional interaction involves the OH···^-O_3S hydrogen bond and links two inversion-related HABS molecules together to form a centrosymmetic $R_2^2(28)$ ring (Figure Supp-1). Formation of this centrosymmetric motif is possible in this structure because both enantiomers of the dye are present. The second-level graph set for **1** (Table Supp-2) includes infinite chains, finite rings, and finite spiral patterns. The spirals arise from combination of the first-level centrosymmetric ring motif with other finite complex interactions (Figure Supp-2).

DL-Lysine/Orange G (2). The racemic nature of this salt allows the formation of centrosymmetric hydrogen-bonded ring motifs, as in **1**. In fact, thirteen ring motifs are found in the first- (Table Supp-3) and second-level (Table Supp-4) graph sets of **2** . In Figure Supp-3 is shown a ring motif generated by hydrogen bonds between the protonated α-amino groups and the carbonyl oxygens of inversion-related lysine molecules in **2**.

L-Lysine/Orange G (3). First-level motifs found in **3** (Table Supp-5) are finite complex patterns except for one infinite pattern, a $C_1^1(9)$ motif defined by side-chain NH_3^+···^-O_3S interactions. No rings are found among either the first- or second-level (Table Supp-6) graph sets. All combinations of two different side-chain NH_3^+···^-O_3S interactions, or one side-chain NH_3^+···^-O_3S and one alpha-NH_3^+···^-O_3S interaction, form chain motifs in **3**. The $C_2^2(10)$ pattern resulting from the combination of two side-chain NH_3^+···^-O_3S interactions is shown in Figure Supp-4. Other patterns involving hydrogen bonds to the side-chain amino group include the two $D_2^2(7)[C_1^1(9)]$ motifs shown in Figure Supp-5.

DL-Histidine/Orange G (4). Although this salt is racemic, no

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centrosymmetric rings are found in the first-level graph set of **4** (Table Supp-7). However, five centrosymmetric ring motifs are observed in the second-level graph set (Table Supp-8). Two of these hydrogen-bonded rings are shown in Figure Supp-6.

L-Histidine/Orange G (5). In **5** the absence of inversion symmetry requires the absence of *centrosymmetric* ring motifs. Only three ring motifs, all non-centrosymmetric, are found in the first-level (Table Supp-9) and second-level (Table Supp-10) graph sets of **5**. One of these rings involves a bifurcated hydrogen bond between a single water proton and two oxygen atoms of a sulfonate group [Figure Supp-7(a)]. Another ring is defined by the linkage of two symmetry-unrelated histidine molecules by hydrogen bonds between the protonated α-amino group and carboxyl oxygen atoms [Figure Supp-7(b)].

TAME/LRO (6). Among the first-level interactions found in **6** (Table Supp-11), only one is infinite: a $\mathbf{C_1^1(11)}$ interaction defined by a hydrogen bond between a guanidinium terminal NH_2 group and a sulfonyl oxygen atom from the tosyl protecting group. The result of this interaction is a winding chain of TAME molecules (Figure Supp-8). In contrast to the first-level interactions, the second-level interactions (Table Supp-12) form predominantly rings and infinite chains. Of special interest is the $\mathbf{R_2^2(8)}$ motif defined by the interaction between the arginine guanidinium group and the sulfonate group of a neighboring dye molecule. The geometries of both functional groups facilitate the elegant bidentate hydrogen-bonding interaction involving the simultaneous "side-on" approach of two guanidinium protons (each from a different terminal NH_2 group) toward two oxygen atoms from this single sulfonate group. This same guanidinium···sulfonate interaction has recently been observed in guanidinium/sulfonate salts designed and characterized by Russell, Etter, and Ward (Ref. 31 in manuscript). Another $\mathbf{R_2^2(8)}$ motif is defined at this same sulfonate group by the hydrogen bonding of two of its oxygen atoms separately to the terminal NH_2 and the side-chain NH groups of another neighboring guanidinium group. The combination of these two bidentate interactions defines an $\mathbf{R_4^3(14)}$ ribbon of molecules extending throughout the crystal structure of **6** (Figure Supp-9).

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Table Supp-1. First-level hydrogen bond graph set motifs for DL-lysine/HABS (1).

Hydrogen Bond Type	Defined Atoms	Motif
a1 = NH_3^+/SO_3^-	N5-H5B···O6	$D_1^1(2)$
a2	N5-H5A···O7	$D_1^1(2)$
a3	N5-H5C···O1	$D_1^1(2)$
b = acid/SO_3^-	O9-H9O···O7	$D_1^1(2)$
c1 = sideNH_3^+/SO_3^-	N6-H6B···O5	$D_1^1(2)$
c2	N6-H6A···O3	$D_1^1(2)$
c3	N6-H6C···O1	$D_1^1(2)$
d = OH/SO_3^-	O4-H4O···O2	$R_2^2(28)$
e = H_2O/SO_3^-	O11W-H11A···O6	$D_1^1(2)$
f = NH_3^+/OH	N5-H5B···O4	$D_1^1(2)$
g = H_2O/acid	O11W-H11W···O10	$D_1^1(2)$
h = sideNH_3^+/OH	N6-H6B···O8	$D_1^1(2)$
i = OH/H_2O	O8-H8O···O11W	$D_1^1(2)$

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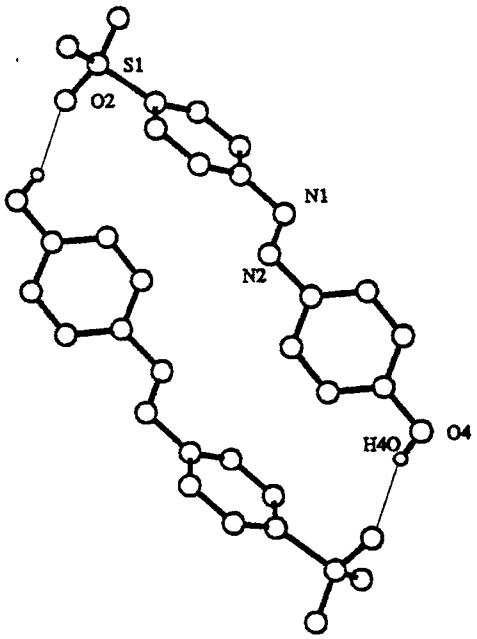

Figure Supp-1. $R_2^2(28)$ motif identified in the first-level graph set of **1**.

Table Supp-2. Two-dimensional matrix listing the second-level hydrogen bond graph set motifs for DL-lysine/HABS (**1**). Letter codes for hydrogen bonds listed on the top row and far left column of the matrix are defined in Table Supp-1. The motif describing the combination of hydrogen bonds a1 and a2, for example, is $R_4^4(12)$.

	a1	a2	a3	b	c1	c2	c3	d	e	f	g	h	i
a1	$D_1^1(2)$	$R_4^4(12)$	$D_2^2(5)$	$C_2^2(9)$	$R_4^4(24)$	$D_2^2(11)$	$D_2^2(11)$	---	$D_2^1(3)$	$D_1^2(3)$	$D_2^2(7)$	$C_2^2(22)$	$D_2^2(16)$
a2		$D_1^1(2)$	$D_2^2(5)$	$R_2^2(14)$	$C_2^2(12)$	$D_2^2(11)$	$D_2^2(11)$	---	$D_2^2(5)$	$D_2^2(5)$	$D_2^2(7)$	$R_4^4(44)$	$D_2^2(16)$
a3			$D_1^1(2)$	$D_2^2(8)$	$D_2^2(11)$	$R_4^4(24)$	$C_2^1(10)$	$D_3^3(19)$ [$R_2^2(28)$]	---	$R_4^4(32)$	$D_2^2(7)$	$D_2^2(11)$	---
b				$D_1^1(2)$	$R_4^4(26)$	$D_2^2(12)$	$D_2^2(12)$	---	$D_2^2(5)$	$D_2^2(8)$	$D_2^2(6)$	$C_2^2(23)$	$D_2^2(16)$
c1					$D_1^1(2)$	$D_2^2(5)$	$D_2^2(5)$	---	$D_2^2(5)$	$D_2^2(11)$	$D_2^2(11)$	$C_1^2(3)$	$D_2^2(16)$
c2						$D_1^1(2)$	$C_2^2(6)$	$D_3^3(19)$ [$R_2^2(28)$]	---	$C_2^2(22)$	$D_2^2(11)$	$D_2^2(5)$	---
c3							$D_1^1(2)$	$D_3^3(19)$ [$R_2^2(28)$]	---	$R_4^4(44)$	$D_2^2(11)$	$D_2^2(5)$	---
d								$R_2^2(28)$	---	$D_3^3(19)$ [$R_2^2(28)$]	---	---	---
e									$D_1^1(2)$	---	$D_2^2(5)$	$D_2^2(15)$	$R_4^4(32)$
f										$D_1^1(2)$	$D_2^2(7)$	$D_2^2(11)$	---
g											$D_1^1(2)$	$D_2^2(11)$	$D_2^2(4)$
h												$D_1^1(2)$	$D_2^2(4)$
i													$D_1^1(2)$

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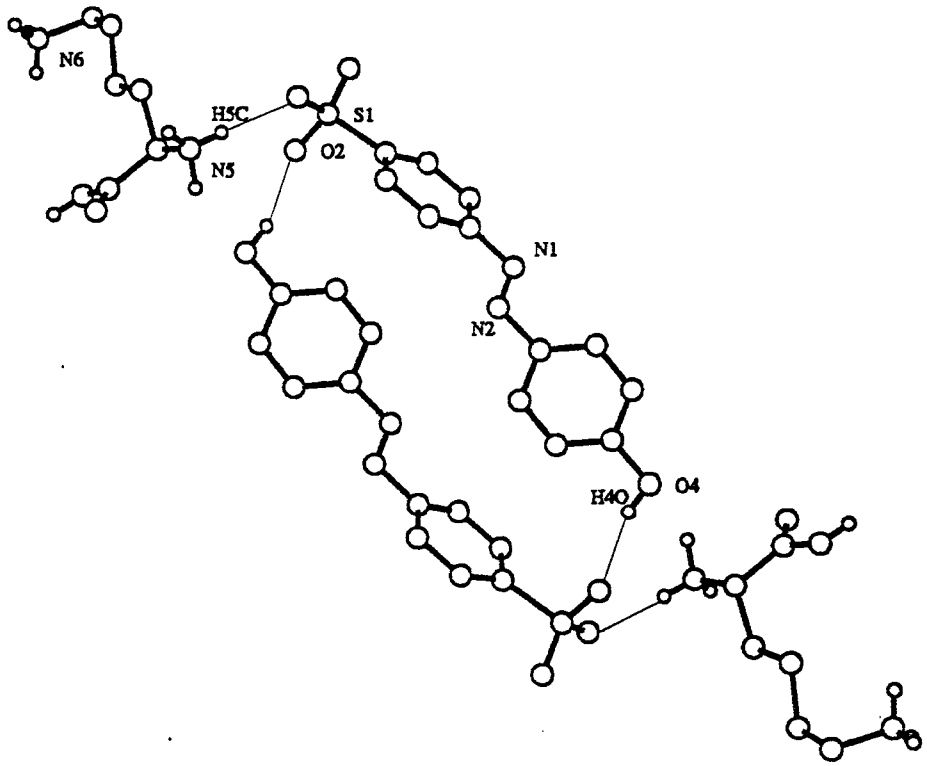

Figure Supp-2. Second-level hydrogen bond motif of **1** generated from two interactions: $NH_3^+\cdots{}^-O_3S$ and $OH\cdots{}^-O_3S$. The $D_3^3(19)[R_2^2(28)]$ motif forms a ring pattern with two inversion-related diad interactions spiraling out from opposite sides of the central ring. Hydrogen bonds are shown as narrow lines.

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Table Supp-3. First-level hydrogen bond graph set motifs for DL-lysine/Orange G (2).

Hydrogen Bond Type	Defined Atoms	Motif
a1 = NH_3^+/SO_3^-	N3-H3A···O1	$D_1^1(2)$
a2	N3-H3B···O5	$D_1^1(2)$
a3	N3-H3C···O4	$D_1^1(2)$
a4	N3-H3C···O5	$D_1^1(2)$
c1 = sideNH_3^+/SO_3^-	N4-H4C···O2	$D_1^1(2)$
c2	N4-H4A···O5	$D_1^1(2)$
e1 = H_2O/SO_3^-	O10W-H10W···O2	$D_1^1(2)$
e2	O11W-H11W···O4	$D_1^1(2)$
e3	O11W-H11A···O3	$D_1^1(2)$
g = H_2O/acid	O9-H9A···O10W	$D_1^1(2)$
s = sideNH_3^+/acid	N4-H4B···O11W	$D_1^1(2)$
t = H_2O/carbonyl	O10W-H10A···O7	$D_1^1(2)$
u = NH_3^+/acid	N3-H3B···O8	$R_2^2(10)$

Table Supp-4. Two-dimensional matrix listing the second-level hydrogen bond graph set motifs for DL-lysine/Orange G (**2**). Letter codes for hydrogen bonds listed on the top row and far left column of the matrix are defined in Table Supp-3. The motif describing the combination of hydrogen bonds a1 and a2, for example, is $R_4^4(20)$.

	a1	a2	a3	a4	c1	c2	e1	e2	e3	g	s	t	u
a1	$D_1^1(2)$	$R_4^4(20)$	$C_2^2(10)$	$C_2^2(10)$	$R_4^4(24)$	$R_2^2(16)$	$D_2^2(5)$	$D_2^2(9)$	$D_2^2(5)$	$D_2^2(8)$	$D_2^2(11)$	$D_2^2(9)$	$D_3^3(10)$ $[R_2^2(10)]$
a2		$D_1^1(2)$	$R_4^4(12)$	$R_4^2(8)$	$R_4^4(16)$	$R_4^2(20)$	$D_2^2(9)$	$D_2^2(5)$	$D_2^2(9)$	$D_2^2(8)$	$D_2^2(11)$	$D_2^2(11)$	$D_3^3(10)$ $[R_2^2(10)]$
a3			$D_1^1(2)$	$R_1^2(4)$	$R_4^4(32)$	$C_2^2(12)$	$D_2^2(9)$	$D_2^1(3)$	$D_2^2(9)$	$D_2^2(8)$	$D_2^2(11)$	$D_2^2(11)$	$D_3^3(10)$ $[R_2^2(10)]$
a4				$D_1^1(2)$	$R_4^4(32)$	$C_2^1(10)$	$D_2^2(9)$	$D_2^2(5)$	$D_2^2(9)$	$D_2^2(8)$	$D_2^2(11)$	$D_2^2(11)$	$D_3^3(10)$ $[R_2^2(10)]$
c1					$D_1^1(2)$	$R_4^4(20)$	$D_2^1(3)$	$D_2^2(9)$	$D_2^2(5)$	$D_2^2(12)$	$D_2^2(5)$	$D_2^2(9)$	$D_3^3(10)$ $[R_2^2(10)]$
c2						$D_1^1(2)$	$D_2^2(9)$	$D_2^2(5)$	$D_2^2(9)$	$D_2^2(12)$	$D_2^2(5)$	$D_2^2(11)$	$D_3^3(10)$ $[R_2^2(10)]$
e1							$D_1^1(2)$	$D_2^2(9)$	$D_2^2(5)$	$D_2^2(4)$	---	$R_4^4(20)$	---
e2								$D_1^1(2)$	$C_2^2(10)$	---	$D_2^2(4)$	$D_2^2(11)$	---
e3									$D_1^1(2)$	---	$D_2^2(4)$	$D_2^2(9)$	---
g										$D_1^1(2)$	$D_2^2(12)$	$D_2^2(4)$	$D_3^3(10)$ $[R_2^2(10)]$
s											$D_1^1(2)$	---	$D_3^3(10)$ $[R_2^2(10)]$
t												$D_1^1(2)$	---
u													$R_2^2(10)$

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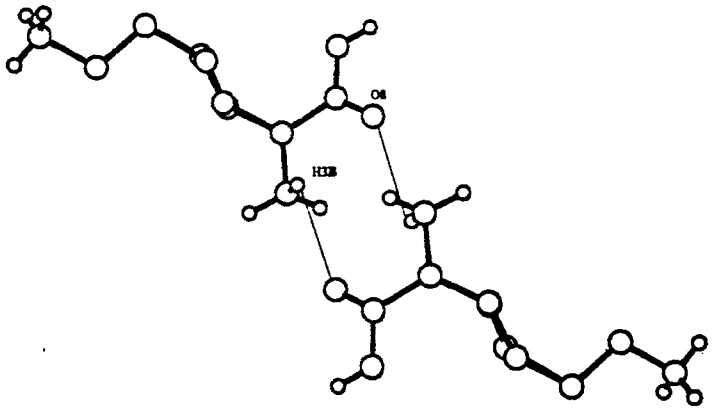

Figure Supp-3. Centrosymmetric $R_2^2(10)$ motif formed from NH_3^+···acid hydrogen bonds between two inversion-related lysine molecules in **2**. Hydrogen bonds are shown as narrow lines.

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Table Supp-5. First-level hydrogen bond graph set motifs for L-lysine/Orange G (3).

Hydrogen Bond Type	Defined Atoms	Motif
a1 = NH_3^+/SO_3^-	N3A-H3CA···O1A	$D_1^1(2)$
a2	N3A-H3BA···O6A	$D_1^1(2)$
a3	N3B-H3BB···O1B	$D_1^1(2)$
b1 = acid/SO_3^-	O9A-H9OA···O5B	$D_1^1(2)$
b2	O9B-H9OB···O5A	$D_1^1(2)$
c1 = sideNH_3^+/SO_3^-	N4A-H4BA···O3A	$D_1^1(2)$
c2	N4A-H4CA···O6A	$D_1^1(2)$
c3	N4B-H4BB···O3B	$D_1^1(2)$
c4	N4B-H4AB···O6B	$D_1^1(2)$
c5	N4B-H4CB···O8B	$C_1^1(9)$
e1 = H_2O/SO_3^-	O11W-H11AW···O2A	$D_1^1(2)$
e2	O11W-H11W···O5A	$D_1^1(2)$
e3	O10W-H10AW···O2B	$D_1^1(2)$
e4	O12W-H···O1B	$D_1^1(2)$
e5	O12W-H···O4B	$D_1^1(2)$
e6	O10W-H10W···O5B	$D_1^1(2)$
g = H_2O/acid	O10W-H10W···O8A	$D_1^1(2)$
j = NH_3^+/H_2O	N3B-H3CB···O10W	$D_1^1(2)$
k1 = NH_3^+/carbonyl	N3A-H3AA···O7B	$D_1^1(2)$
k2	N3B-H3AB···O7A	$D_1^1(2)$
r = sideNH_3^+/acid	N4A-H4AA···O8B	$D_1^1(2)$
s1 = sideNH_3^+/H_2O	N4B-H4CB···O11W	$D_1^1(2)$
s2	N4A-H4AA···O10W	$D_1^1(2)$

Table Supp-6. Two-dimensional matrix listing the second-level hydrogen bond graph set motifs for L-lysine/Orange G (3). Letter codes for hydrogen bonds listed on the top row and far left column of the matrix are defined in Table . The motif describing the combination of hydrogen bonds a1 and a2, for example, is $C_2^2(10)$.

	a1	a2	a3	b1	b2	c1	c2	c3	c4	e1	e2	e3	e4	e5	e6	g	j	k1	k2	r1	r2	s1	s2
a1	$D_1^1(2)$	$C_2^2(10)$	—	$D_2^2(8)$	$D_2^2(9)$	$C_2^2(12)$	$C_2^2(16)$	—	—	$D_2^2(5)$	$D_2^2(9)$	—	—	—	—	$D_2^2(7)$	—	$D_2^2(5)$	$D_2^2(9)$	$D_2^2(11)$	—	—	$D_2^2(11)$
a2		$D_1^1(2)$	$D_2^2(5)$	$D_2^2(8)$	$D_2^2(5)$	$C_2^2(16)$	$C_2^1(10)$	—	—	$D_2^2(9)$	$D_2^2(5)$	—	—	—	$D_2^2(7)$	$D_2^2(7)$	—	$D_2^2(5)$	—	$D_2^2(11)$	—	—	$D_2^2(11)$
a3			$D_1^1(2)$	$D_2^2(9)$	$D_2^2(8)$	—	—	$C_2^2(12)$	$C_2^2(16)$	—	—	—	—	$D_2^2(9)$	—	—	$D_2^2(5)$	—	$D_2^2(5)$	$D_2^2(7)$	$C_1^1(9)$ $[D_1^1(2)]$	$D_2^2(11)$	—
b1				$D_1^1(2)$	—	$D_2^2(12)$	$D_2^2(12)$	$D_2^2(9)$	$D_2^1(3)$	—	—	—	—	$D_2^2(5)$	$D_2^2(5)$	$D_2^2(6)$	—	$C_2^2(15)$	—	$D_2^2(12)$	—	—	$D_2^2(12)$
b2					$D_1^1(2)$	$D_2^2(9)$	$D_2^2(5)$	$D_2^2(12)$	$D_2^2(12)$	$D_2^2(9)$	$D_2^1(3)$	—	—	—	—	—	$D_2^2(8)$	—	$C_2^2(15)$	$D_2^2(6)$	$C_1^1(9)$ $[D_1^1(2)]$	$D_2^2(12)$	—
c1						$D_1^1(2)$	$C_2^2(10)$	—	—	$D_2^2(5)$	$D_2^2(9)$	—	—	—	—	$D_2^2(11)$	—	$D_2^2(11)$	$D_2^2(9)$	$D_2^2(5)$	—	—	$D_2^2(5)$
c2							$D_1^1(2)$	—	—	$D_2^2(9)$	$D_2^2(5)$	—	—	—	—	$D_2^2(11)$	—	$D_2^2(11)$	$D_2^2(11)$	$D_2^2(5)$	—	—	$D_2^2(5)$
c3								$D_1^1(2)$	$C_2^2(10)$	—	—	—	—	$D_2^2(9)$	$D_2^2(9)$	—	$D_2^2(11)$	$D_2^2(9)$	$D_2^2(11)$	$D_2^2(11)$	$C_1^1(9)$ $[D_1^1(2)]$	$D_2^2(5)$	—
c4									$D_1^1(2)$	—	—	$D_2^2(9)$	$D_2^2(9)$	$D_2^2(5)$	$D_2^2(5)$	—	$D_2^2(11)$	$D_2^2(11)$	$D_2^2(11)$	$D_2^2(11)$	$C_1^1(9)$ $[D_1^1(2)]$	$D_2^2(5)$	—
e1										$D_1^1(2)$	$C_2^2(10)$	—	—	—	—	—	—	—	$D_2^2(9)$	—	—	$D_2^2(4)$	—
e2											$D_1^1(2)$	—	—	—	—	—	—	—	$D_2^2(11)$	—	—	$D_2^2(4)$	—
e3												$D_1^1(2)$	$D_2^2(5)$	$D_2^2(9)$	$C_2^2(10)$	$D_2^2(5)$	$D_2^2(4)$	$D_2^2(9)$	—	—	—	—	$D_2^2(4)$
e4													$D_1^1(2)$	$C_2^2(10)$	$D_2^2(9)$	—	—	$D_2^2(9)$	—	—	—	—	—
e5														$D_1^1(2)$	$D_2^2(5)$	—	—	$D_2^2(11)$	—	—	—	—	—
e6															$D_1^1(2)$	$D_2^2(3)$	$D_2^2(4)$	$D_2^2(11)$	—	—	—	—	$D_2^2(4)$
g																$D_1^1(2)$	$D_2^2(4)$	$D_2^2(7)$	—	$D_2^2(11)$	—	—	$D_2^2(11)$
j																	$D_1^1(2)$	—	$D_2^2(5)$	$D_2^2(7)$	$C_1^1(9)$ $[D_1^1(2)]$	$D_2^2(11)$	$D_2^1(3)$
k1																		$D_1^1(2)$	—	$D_2^2(11)$	—	—	$D_2^2(11)$
k2																			$D_1^1(2)$	$D_2^2(7)$	$C_1^1(9)$ $[D_1^1(2)]$	$D_2^2(11)$	—
r1																				$D_1^1(2)$	$C_1^1(9)$ $[D_1^1(2)]$	$D_2^2(11)$	—
r2																					$C_1^1(9)$	$C_1^1(9)$ $[D_1^1(2)]$	—
s1																						$D_1^1(2)$	—
s2																							$D_1^1(2)$

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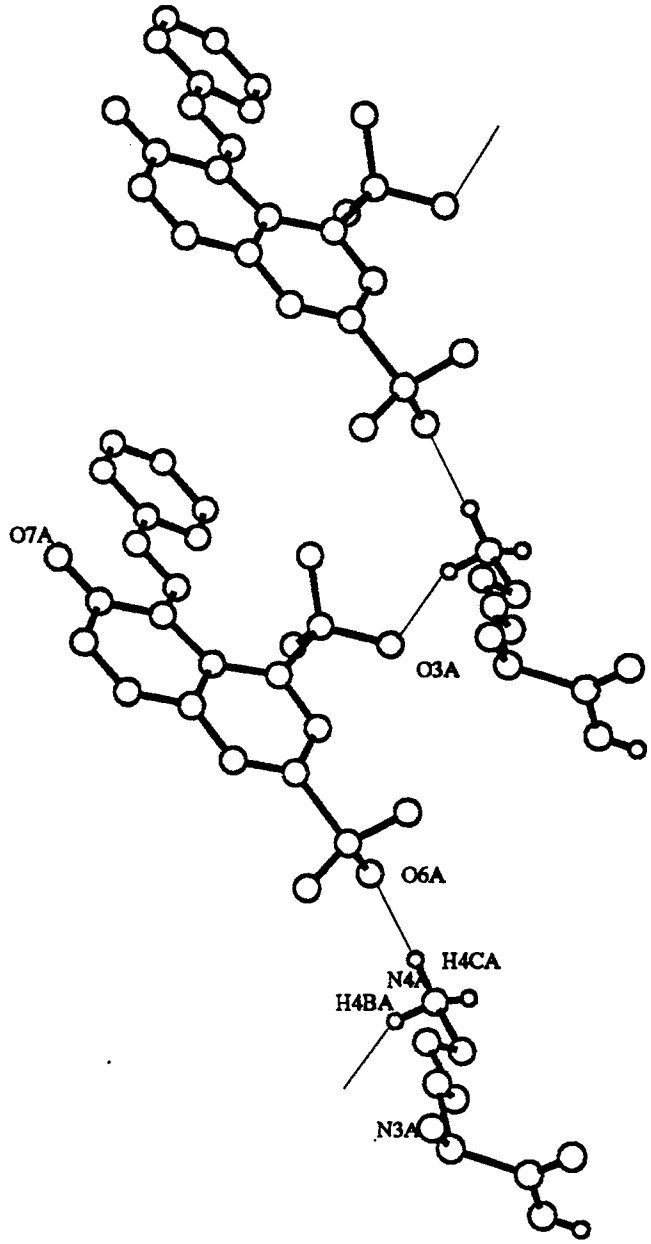

Figure Supp-4. A second-level $C_2^2(10)$ motif of **3** formed from the combination of two side-chain NH_3^+···sulfonate hydrogen bonds, shown as narrow lines.

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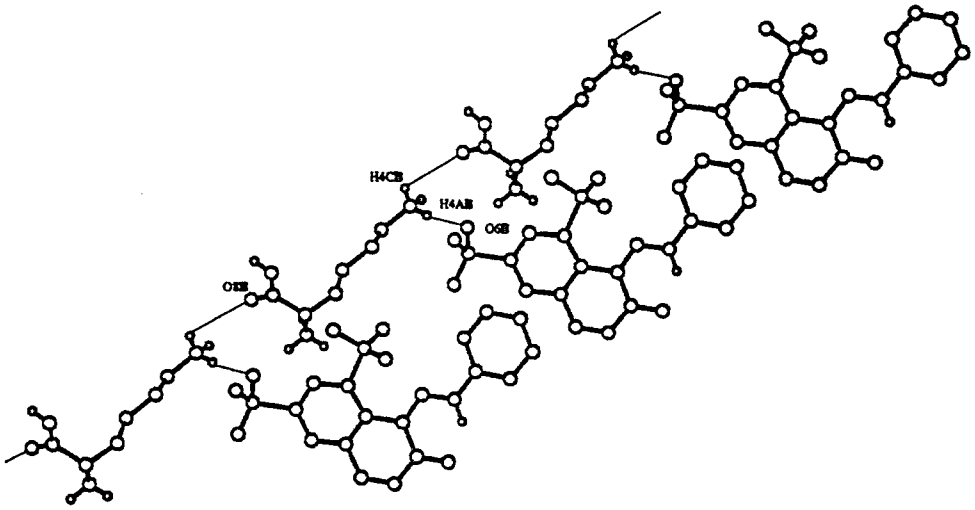
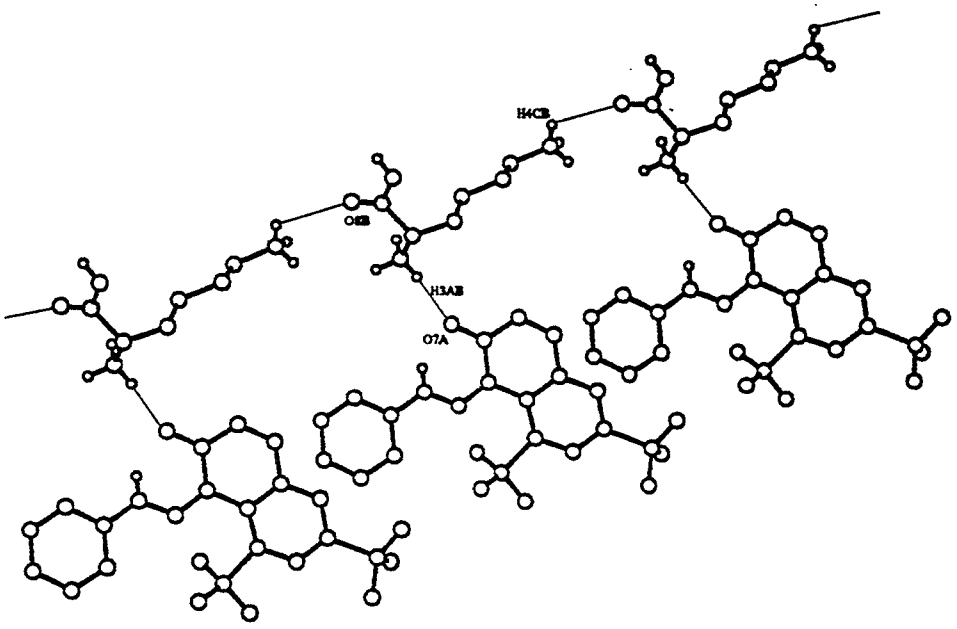


(a)



(b)

Figure Supp-5. Two second-level hydrogen bond graph set motifs found in **3** which involve side-chain NH_3^+ hydrogen bonds. (a) $D_2^2(7)[C_1^1(9)]$ motif generated from NH_3^+···acid and NH_3^+···sulfonate interactions. (b) $D_2^2(7)[C_1^1(9)]$ motif resulting from NH_3^+···acid and α-NH_3^+···carbonyl interactions.

J2142-14

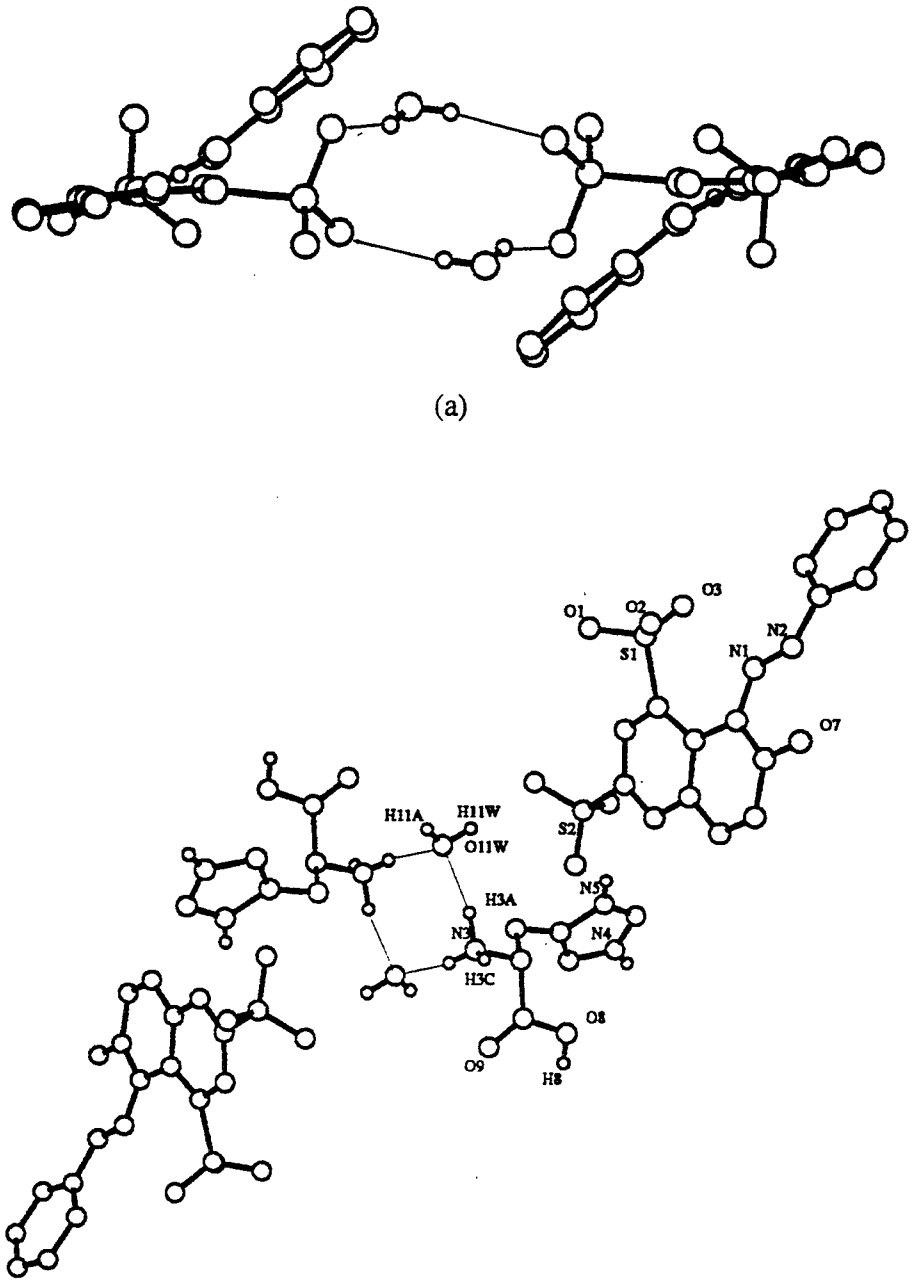
Table Supp-7. First-level hydrogen bond graph set motifs for DL-histidine/Orange G (4).

Hydrogen Bond Type	Defined Atoms	Motif
a = NH_3^+/SO_3^-	N3-H3C···O6	$D_1^1(2)$
b = acid/SO_3^-	O8-H8···O2	$D_1^1(2)$
e1 = H_2O/SO_3^-	O12W-H12W···O5	$D_1^1(2)$
e2	O12W-H12A···O3	$D_1^1(2)$
e3	O10W-H10A···O1	$D_1^1(2)$
e4	O11W-H11W···O5	$D_1^1(2)$
e5	O10W-H10W···O1	$D_1^1(2)$
e6	O10W-H10W···O3	$D_1^1(2)$
j1 = NH_3^+/H_2O	N3-H3A···O11W	$D_1^1(2)$
j2	N3-H3C···O11W	$D_1^1(2)$
k = NH_3^+/carbonyl	N3-H3B···O7	$D_1^1(2)$
l = sideNH/SO_3^-	N5-H5N···O6	$D_1^1(2)$
m = sideNH/H_2O	N4-H4N···O12W	$D_1^1(2)$

Table Supp-8. Two-dimensional matrix listing the second-level hydrogen bond graph set motifs for DL-histidine/Orange G (**4**). Letter codes for hydrogen bonds listed on the top row and far left column of the matrix are defined in Table Supp-7. The motif describing the combination of hydrogen bonds a and b, for example, is $C_2^2(13)$.

	a	b	e1	e2	e3	e4	e5	e6	j1	j2	k	l	m
a	$D_1^1(2)$	$C_2^2(13)$	$D_2^2(5)$	---	---	$D_2^2(5)$	---	---	$D_2^2(5)$	$D_2^2(5)$	$C_2^2(12)$	$C_2^1(8)$	$D_2^2(10)$
b		$D_1^1(2)$	$D_2^2(9)$	$D_2^2(5)$	$D_2^2(5)$	$D_2^2(9)$	$D_2^2(5)$	$D_2^2(5)$	$D_2^2(8)$	$D_2^2(8)$	$D_2^2(8)$	$C_2^2(15)$	$D_2^2(11)$
e1			$D_1^1(2)$	$C_2^2(10)$	---	$D_2^1(3)$	---	$D_2^2(9)$	---	---	---	$D_2^2(5)$	---
e2				$D_1^1(2)$	$D_2^2(5)$	---	$D_2^2(5)$	$D_2^1(3)$	---	---	$D_2^2(9)$	$D_2^2(9)$	$D_2^2(4)$
e3					$D_1^1(2)$	---	$R_4^2(8)$	$R_4^4(12)$	---	---	$D_2^2(9)$	$D_2^2(9)$	---
e4						$D_1^1(2)$	$D_2^2(9)$	$D_2^2(9)$	$D_2^2(4)$	$D_2^2(4)$	$D_2^2(11)$	$D_2^2(5)$	---
e5							$D_1^1(2)$	$R_1^2(4)$	---	---	$D_2^2(9)$	$D_2^2(9)$	---
e6								$D_1^1(2)$	---	---	$D_2^2(9)$	$D_2^2(9)$	---
j1									$D_1^1(2)$	$R_4^2(8)$	$D_2^2(5)$	$D_2^2(9)$	$D_2^2(10)$
j2										$D_1^1(2)$	$D_2^2(5)$	$D_2^2(9)$	$D_2^2(10)$
k											$D_1^1(2)$	$R_4^4(32)$	$D_2^2(10)$
l												$D_1^1(2)$	$D_2^2(7)$
m													$D_1^1(2)$

J2142-16



(a)

(b)

Figure Supp-6. Ring motifs found in the second-level hydrogen bond graph set of **4**. (a) $R_4^4(12)$ motif composed of two pairs of symmetry-related hydrogen bonds between water molecules and sulfonate oxygen atoms. (b) $R_4^2(8)$ motif formed by symmetry-related hydrogen bonds between amino groups and water molecules. Hydrogen bonds are shown as narrow lines.

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Table Supp-9. First-level hydrogen bond graph set motifs for L-histidine/Orange G (5).

Hydrogen Bond Type	Defined Atoms	Motif
a1 = NH_3^+/SO_3^-	N3B-H3AB···O5A	$D_1^1(2)$
a2	N3A-H3AA···O5B	$D_1^1(2)$
a3	N3A-H3BA···O6A	$D_1^1(2)$
a4	N3B-H3BB···O1A	$D_1^1(2)$
e1 = H_2O/SO_3^-	O13W-H13W···O1B	$D_1^1(2)$
e2	O15W-H···O1A	$D_1^1(2)$
e3	O10W-H10AW···O3A	$D_1^1(2)$
e4	O12W-H12W···O3B	$D_1^1(2)$
e5	O11W-H11W···O4B	$D_1^1(2)$
e6	O14W-H14AW···O2A	$D_1^1(2)$
e7	O14W-H14W···O4A	$D_1^1(2)$
e8	O12W-H···O6B	$D_1^1(2)$
e9	O11W-H11AW···O2B	$D_1^1(2)$
e10	O10W-H10W···O6A	$D_1^1(2)$
e11	O12W-H···O4B	$D_1^1(2)$
e12	O10W-H10W···O4A	$D_1^1(2)$
g1	O8B-H8B···O11W	$D_1^1(2)$
g2 = H_2O/acid	O14W-H···O8A	$D_1^1(2)$
g3	O13W-H···O9A	$D_1^1(2)$
j	N3B-H3CB···O13W	$D_1^1(2)$
m1 = NH_3^+/H_2O	N5B-H5NB···O12W	$D_1^1(2)$
m2	N5A-H5NA···O10W	$D_1^1(2)$
u1 = NH_3^+/acid	N3A-H3CA···O9B	$D_1^1(2)$
u2	N3B-H3BB···O8A	$D_1^1(2)$
w1 = H_2O/H_2O	O15W-H···O12W	$D_1^1(2)$
w2	O13W-H···O10W	$D_1^1(2)$
v1 = sideNH/carbonyl	N4A-H4NA···O7A	$D_1^1(2)$
v2	N4B-H4NB···O7B	$D_1^1(2)$

Table Supp-10. Two-dimensional matrix listing the second-level hydrogen bond graph set motifs for L-histidine/Orange G (**5**). Letter codes for hydrogen bonds listed on the top row and far left column of the matrix are defined in Table Supp-4. The motif describing the combination of hydrogen bonds a1 and a3, for example, is $D_2^2(5)$.

	a1	a2	a3	a4	e1	e2	e3	e4	e5	e6	e7	e8	e9	e10	e11	e12
a1	$D_1^1(2)$	—	$D_2^2(5)$	$C_2^2(10)$	—	—	$D_2^2(9)$	—	—	$D_2^2(9)$	$D_2^2(5)$	—	—	$D_2^2(5)$	—	$D_2^2(5)$
a2		$D_1^1(2)$	$D_2^2(5)$	—	$D_2^2(9)$	—	—	$D_2^2(9)$	$D_2^2(5)$	—	—	$D_2^2(5)$	$D_2^2(9)$	—	$D_2^2(5)$	—
a3			$D_1^1(2)$	$D_2^2(9)$	—	$D_2^2(9)$	$D_2^2(9)$	—	—	$D_2^2(9)$	$D_2^2(5)$	—	—	$D_2^1(3)$	—	$D_2^2(5)$
a4				$D_1^1(2)$	—	$D_2^1(3)$	$D_2^2(5)$	—	—	$D_2^2(5)$	$D_2^2(9)$	—	—	$D_2^2(9)$	—	$D_2^2(9)$
e1					$D_1^1(2)$	—	—	—	—	—	—	$D_2^2(9)$	$D_2^2(5)$	—	$D_2^2(9)$	—
e2						$D_1^1(2)$	$D_2^2(5)$	—	—	$D_2^2(5)$	$D_2^2(9)$	—	—	$D_2^2(9)$	—	$D_2^2(9)$
e3							$D_1^1(2)$	—	—	$D_2^2(5)$	$D_2^2(9)$	—	—	$C_2^2(10)$	—	$C_2^2(10)$
e4								$D_1^1(2)$	$D_2^2(9)$	—	—	$C_2^2(10)$	$D_2^2(5)$	—	$C_2^2(10)$	—
e5									$D_1^1(2)$	—	—	$D_2^2(5)$	$C_2^2(10)$	—	$D_2^1(3)$	—
e6										$D_1^1(2)$	$C_2^2(10)$	—	—	$D_2^2(9)$	—	$D_2^2(9)$
e7											$D_1^1(2)$	—	—	$D_2^2(5)$	—	$D_2^1(3)$
e8												$D_1^1(2)$	$D_2^2(9)$	—	$R_1^2(4)$	—
e9													$D_1^1(2)$	—	$D_2^2(9)$	—
e10														$D_1^1(2)$	—	$R_1^2(4)$
e11															$D_1^1(2)$	—
e12																$D_1^1(2)$

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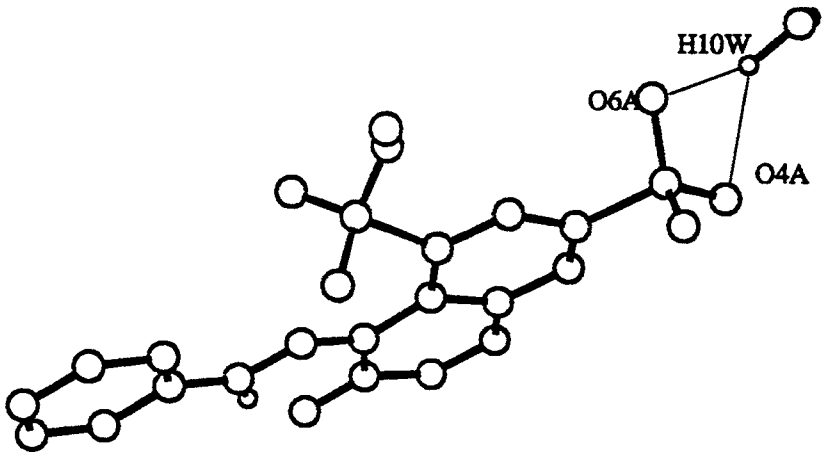
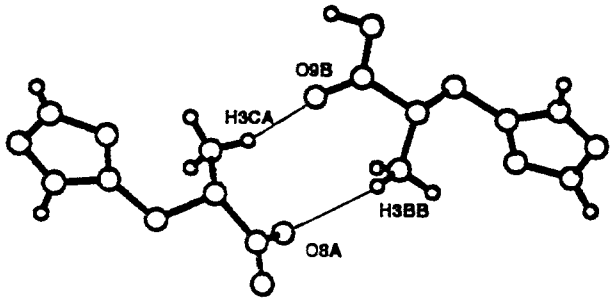
Table Supp-16. (Continued) Second-level hydrogen bond graph sets for L-histidine/Orange G (**5**). Letter codes for hydrogen bonds are defined in Table Supp-9.

	g1	g2	g3	j	m1	m2	u1	u2	v1	v2	w1	w2
a1	$D_2^2(8)$	–	–	$D_2^2(5)$	$D_2^2(9)$	–	$D_2^2(7)$	$D_2^2(5)$	$D_2^2(11)$	$D_2^2(10)$	–	–
a2	–	$D_2^2(7)$	–	–	–	–	–	–	$D_2^2(10)$	$D_2^2(11)$	–	–
a3	–	$D_2^2(8)$	$D_2^2(7)$	–	–	$D_2^2(9)$	$D_2^2(5)$	$D_2^2(7)$	$C_2^2(17)$	–	–	–
a4	$D_2^2(8)$	–	–	$D_2^2(5)$	$D_2^2(9)$	–	$D_2^2(7)$	–	$D_2^2(9)$	$D_2^2(10)$	–	–
e1	–	–	$D_2^2(5)$	$D_2^2(4)$	–	–	–	–	–	$D_2^2(9)$	–	$D_2^2(5)$
e2	–	–	–	–	–	–	–	–	$D_2^2(9)$	–	$D_2^2(5)$	–
e3	–	–	–	–	–	$D_2^2(4)$	–	–	$D_2^2(9)$	–	–	$D_2^2(4)$
e4	–	–	–	–	$D_2^2(4)$	–	–	–	–	$D_2^2(9)$	$D_2^2(5)$	–
e5	$D_2^2(4)$	–	–	–	–	–	–	–	–	$D_2^2(11)$	–	–
e6	–	$D_2^2(5)$	–	–	–	–	–	–	$D_2^2(5)$	–	–	–
e7	–	$D_2^2(4)$	–	–	–	–	–	–	$D_2^2(11)$	–	–	–
e8	–	–	–	–	$D_2^2(5)$	–	–	–	–	$D_2^2(5)$	–	–
e9	$D_2^2(4)$	–	–	–	–	–	–	–	–	$D_2^2(9)$	–	–
e10	–	–	–	–	–	$D_2^2(4)$	–	–	$D_2^2(11)$	–	–	$D_2^2(4)$
e11	–	–	–	–	$D_2^2(5)$	–	–	–	–	$D_2^2(5)$	$D_2^2(5)$	–
e12	–	–	–	–	–	$D_2^2(4)$	–	–	$D_2^2(11)$	–	–	$D_2^2(4)$
g1	$D_1^1(2)$	–	–	$D_2^2(8)$	$D_2^2(10)$	–	$D_2^2(6)$	$D_2^2(8)$	–	$D_2^2(11)$	–	–
g2		$D_1^1(2)$	$D_2^2(6)$	–	–	$D_2^2(10)$	$D_2^2(8)$	$D_2^2(4)$	$D_2^2(11)$	–	–	–
g3			$D_1^1(2)$	$D_2^2(4)$	–	$D_2^2(9)$	$D_2^2(7)$	$D_2^2(5)$	$D_2^2(10)$	–	–	$D_1^2(3)$
j				$D_1^1(2)$	$D_2^2(9)$	–	$D_2^2(7)$	$D_2^2(5)$	–	$D_2^2(10)$	–	$D_2^2(4)$
m1					$D_1^1(2)$	–	$D_2^2(9)$	$D_2^2(9)$	–	$D_2^2(7)$	$D_2^2(4)$	–
m2						$D_1^1(2)$	$D_2^2(9)$	$D_2^2(9)$	$D_2^2(7)$	–	–	$D_2^1(3)$
u1							$D_1^1(2)$	$R_2^2(10)$	$D_2^2(10)$	$D_2^2(10)$	–	–
u2								$D_1^1(2)$	$D_2^2(10)$	$D_2^2(10)$	–	–
v1									$D_1^1(2)$	–	–	–
v2										$D_1^1(2)$	–	–
w1											$D_1^1(2)$	–
w2												$D_1^1(2)$

J2142-20



(a)



(b)

Figure Supp-7. Some ring motifs found in the second-level hydrogen bond graph set of 5. (a) $R_1^2(4)$ motif resulting from a bifurcated hydrogen bond between a water proton and sulfonate oxygen atoms. (b) $R_2^2(10)$ motif composed of two symmetry-unrelated histidine molecules linked by $NH_3^+\cdots$acid hydrogen bonds which are shown as narrow lines.

J2142-21

Table Supp-11. First-level hydrogen bond graph set motifs for tosyl arginine methyl ester/Little Rock Orange (6).

Hydrogen Bond Type	Defined Atoms	Motif
n1 = sideNH_2/SO_3^-	N5-H5A···O3	$D_1^1(2)$
n2	N4-H4A···O1	$D_1^1(2)$
n3	N5-H5N···O2	$D_1^1(2)$
o = sideNH/SO_3^-	N3-H3N···O1	$D_1^1(2)$
p = α-NH_2/SO_3^-	N6-H6N···O2	$D_1^1(2)$
q = sideNH_2/SO_2	N4-H4N···O8	$C_1^1(11)$

J2142-22

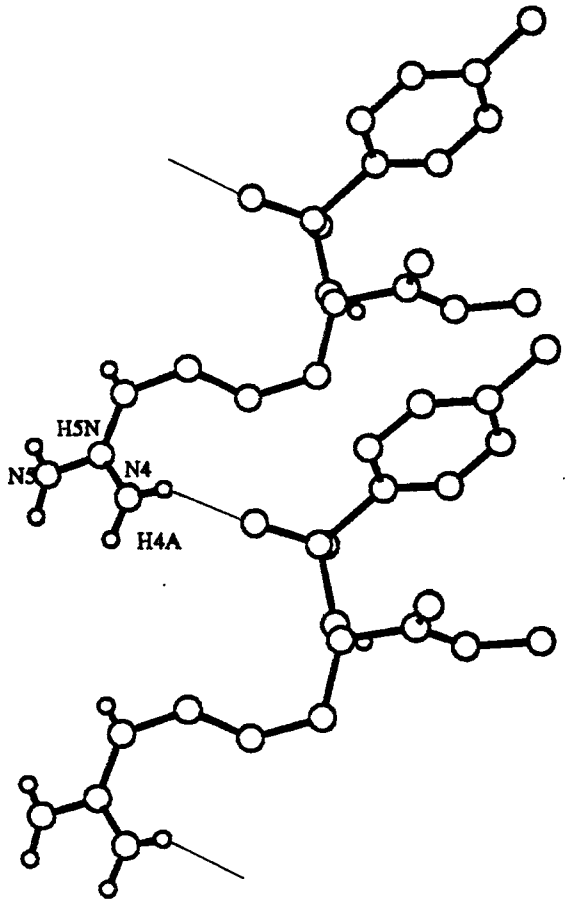


Figure Supp-8. $C_1^1(11)$ chain formed in **6** as a result of $NH_2\cdots O_2S$ hydrogen bond interactions throughout the crystal. Hydrogen bonds are shown as narrow lines.

J2142-23

Table Supp-II. Two-dimensional matrix listing the second-level hydrogen bond graph set motifs for tosyl arginine methyl ester/Little Rock Orange (**6**). Letter codes for hydrogen bonds listed on the top row and far left column of the matrix are defined in Table Supp-II. The motif describing the combination of hydrogen bonds n1 and n2, for example, is $R_2^2(8)$.

	n1	n2	n3	o	p	q
n1	$D_1^1(2)$	$R_2^2(8)$	$C_2^2(6)$	$C_2^2(8)$	$C_2^2(13)$	$C_1^1(11)$ $[D_1^1(2)]$
n2		$D_1^1(2)$	$C_2^2(8)$	$C_2^1(6)$	$C_2^2(13)$	$C_1^1(11)$ $[D_1^1(2)]$
n3			$D_1^1(2)$	$R_2^2(8)$	$C_2^1(11)$	$C_1^1(11)$ $[D_1^1(2)]$
o				$D_1^1(2)$	$C_2^2(11)$	$C_1^1(11)$ $[D_1^1(2)]$
p					$D_1^1(2)$	$C_1^1(11)$ $[D_1^1(2)]$
q						$D_1^1(2)$

J2142-24

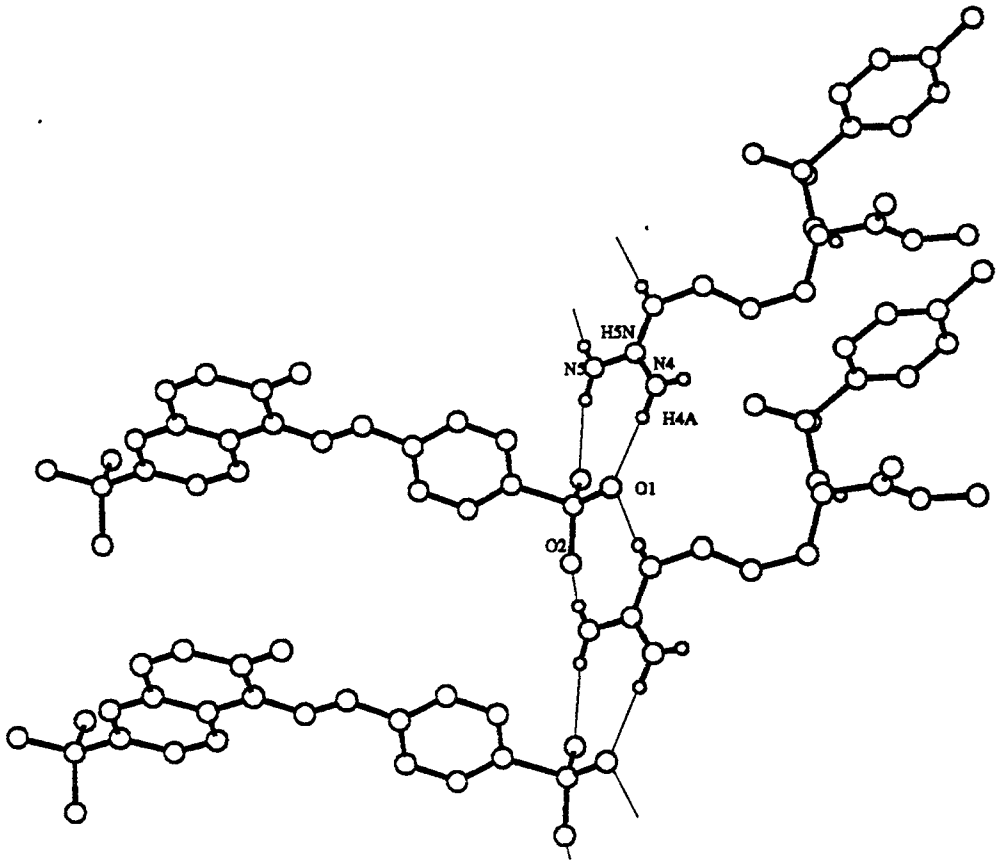


Figure Supp-9. A two-dimensional hydrogen-bonded ribbon motif found in 6. The $R_4^3(14)$ ribbon is formed by combining two adjacent $R_2^2(8)$ motifs. The rings are composed of guanidinium···sulfonate hydrogen bonds between the side chains of arginine molecules and nearby sulfonate groups. Hydrogen bonds are shown as narrow lines.

J2142-25

Additional Experimental Details for Crystal Structure Determinations

Ordered non-hydrogen atoms were refined anisotropically in all six structures. In DL-lysine/Orange G (**2**), peaks found in difference maps suggested disorder in the lysine side chain. This disorder was modeled by assigning fixed partial occupancies of 0.8 to the two disordered methylene carbons C(17) and C(18) at their more populated positions (and refining these atoms anisotropically) and placing carbons C(17A) and C(18A) with occupancies of 0.2 at the less populated positions (and refining these atoms isotropically). Additional peaks in the difference maps suggested that the α-amino group and the S(2) sulfonate group might be disordered as well. Attempts to model this disorder (using two different positions for the α-amino group and two different rotational orientations of the SO_3 group) did not lead to significant improvement in the structure and were therefore not pursued. In L-lysine/Orange G (**3**), the O(12W) water molecule site was only partially occupied. Positional parameters, isotropic B and multiplicity were refined, resulting in a site occupancy of 37%. In L-histidine/Orange G (**5**), the site of O(15W) was partially occupied; positional parameters, isotropic B and multiplicity were refined, resulting in a site occupancy of 50%.

Hydrogen atom positional parameters were refined unless this led to unreasonable bond lengths. All hydrogen atoms were refined with fixed thermal parameters (approximately 1.2 times the isotropic equivalent of the attached atom) in structures **1**, **3**, **4**, and **6**. In structure **2**, hydrogens bonded to carbons were placed in calculated positions and were not refined. Hydrogens bonded to the lysine amino groups failed to refine and so were included in fixed positions at difference map locations. The remaining hydrogens in the structure were refined with fixed thermal parameters. In structure **5** it was not possible to locate all the α–amino hydrogens unambiguously, so one hydrogen at each α–amino group was located in the difference map and used as a guide in placing the other α–amino hydrogens in calculated positions. Hydrogen atoms bonded to the other heteroatoms in this structure were refined with thermal parameters fixed at approximately 1.2 times the isotropic equivalent of the attached atom, while hydrogen atoms bonded to carbons were placed in calculated positions and were

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not refined.

Absorption corrections were made using either the program *DIFABS* [1] or the psi scan technique.[2] Where warranted, a correction for secondary extinction was applied.[3] Cell parameters and further details of the data collection, structure solution, and refinement are given in Table Supp-13.

(1) Walker, N.; Stuart, D. *Acta Crystallogr.* **1983**, *A39*, 158-166.

(2) North, A. C. T.; Phillips, D. C.; Mathews, F. S. *Acta Crystallogr.* **1968**, *A24*, 351-359.

(3) Zachariasen, W. H. *Acta Crystallogr.* **1963**, *16*, 1139-1144.

J2142-27

Table Supp-13. Cell data, data collection parameters, and refinement results for DL-lysine/HABS (**1**), DL-lysine/Orange G (**2**), L-lysine/Orange G (**3**), DL-histidine/Orange G (**4**), L-histidine/Orange G (**5**), and tosyl arginine methyl ester/Little Rock Orange (**6**)

Crystal Data	(1)	(2)	(3)
No. of amino acid molecules*	1	1	2
No. of dye molecules*	2	1	2
No. of water molecules*	1	2	3
Crystal system	triclinic	triclinic	monoclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P2_1$
a (Å)	8.282(1)	10.398(2)	8.973(2)
b (Å)	12.513(2)	15.508(2)	28.989(2)
c (Å)	17.044(2)	8.704(2)	10.539(1)
α (°)	72.626(1)	97.16(1)	90
β (°)	77.647(1)	99.63(1)	113.93(1)
γ (°)	84.358(1)	99.75(1)	90
V ($Å^3$)	1645.6(5)	1346.7(4)	2505.8(8)
Z	2	2	4
M_r	720.77	590.62	581.61
D_x (g cm^{-3})	1.454	1.456	1.541
Dimensions (mm)	0.24 X 0.16 X 0.08	0.52 X 0.40 X 0.08	0.35 X 0.10 X 0.10
F(000)	756	620	1220

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μ (cm^{-1})	20.20	23.18	24.68
Data collection			
Temperature (K)	298	173	173
Number of cell reflections; 2θ range (°)	25; 40.0-52.0	25; 49.2-49.9	25; 31.0-46.5
$2\theta_{max}$ (°)	139.8	140.3	140.2
No. of reflections measured	5409	7797	7366
No. of unique reflections	5203	4963	7052
No. of observed reflections	3929	4154	5536
R_{int}	0.042	0.034	0.025
Absorption correction	*DIFABS*	psi scans	psi scans
Trans. factors	0.89-1.08	0.60-1.00	0.93-1.00
Structure Refinement			
No. of parameters	551	378	857
R; wR	0.035; 0.043	0.051; 0.064	0.031; 0.032
$(\Delta/\sigma)_{max}$	0.00	0.04	0.04
$\Delta\rho$ (e $Å^{-3}$)	-0.27-0.20	-0.37-0.74	-0.25-0.24
S	1.61	3.64	1.47
Extinction coefficient	0.16820×10^{-5}	-----	-----
Decay correction	None	None	4.10% decl.

J214/2-29

Crystal Data	(4)	(5)	(6)
No. of amino acid molecules*	1	2	1
No. of dye molecules*	1	2	1
No. of water molecules*	3	6	0
Crystal system	triclinic	triclinic	orthorhombic
Space group	$P\bar{1}$	P1	$P2_12_12_1$
a (Å)	8.243(1)	9.206(1)	7.573(1)
b (Å)	11.981(2)	10.917(2)	14.410(1)
c (Å)	14.392(1)	14.526(2)	32.722(3)
α (°)	111.40(1)	101.30(1)	90
β (°)	94.21(1)	90.59(1)	90
γ (°)	89.82(1)	113.25(1)	90
V ($Å^3$)	1319.2(6)	1309.2(8)	3571(1)
Z	2	2	4
M_r	617.60	617.60	726.86
D_x (g cm^{-3})	1.555	1.566	1.352
Dimensions (mm)	0.48 X 0.19 X 0.10	0.55 X 0.32 X 0.28	0.27 X 0.08 X 0.11
F(000)	644	644	1536
μ (cm^{-1})	24.36	24.54	18.01
Data collection			
Temperature (K)	298	173	173

J2142-30

Number of cell reflections; 2θ range (°)	25; 40.0-52.0	25; 40.0-52.0	25; 40.0-50.0
$2\theta_{max}$ (°)	139.9	139.9	139.7
No. of reflections measured	5030	7492	6982
No. of unique reflections	4821	4747	6641
No. of observed reflections	3636	4527	5155
R_{int}	0.031	0.026	0.038
Absorption correction	*DIFABS*	*DIFABS*	psi scans
Trans. factors	0.67-1.58	0.83-1.26	0.91-1.00
Structure Refinement			
No. of parameters	452	777	577
R; wR	0.047; 0.058	0.040; 0.052	0.041; 0.044
$(\Delta/\sigma)_{max}$	0.07	0.38	0.05
$\Delta\rho$ (e Å^{-3})	-0.54-0.51	-0.42-0.80	-0.29-0.31
S	2.19	2.41	1.32
Extinction coefficient	0.17620×10^{-5}	-----	-----
Decay correction	16.00% decl.	None	None

*in the asymmetric unit

All structures:

Criterion for observed reflection: $I > 3\sigma(I)$

Function minimized: $\Sigma w(|F_{obs}| - |F_{calc}|)^2$ where $w = 4F_{obs}^2/\sigma^2(F_{obs}^2)$

$R = \Sigma(|F_{obs}| - |F_{calc}|)/\Sigma|F_{obs}|$; $wR = [\Sigma w(|F_{obs}| - |F_{calc}|)^2/\Sigma w|F_{obs}|^2]^{1/2}$

J2142-31

$R_{int} = \Sigma\Sigma|\langle F_i^2\rangle - F_{ij}^2|/\Sigma m\langle F_i^2\rangle$

S = Goodness of Fit = $[\Sigma(|F_{obs}| - |F_{calc}|)/\sigma](n - m)^{-1}$

Positional parameters and B(eq) for HABS/DL-Lysine J2142-32

atom	x	y	z	B(eq)
S(1)	0.37559(7)	0.85374(5)	0.13235(4)	2.57(4)
S(2)	0.39135(7)	0.36590(5)	0.14934(4)	2.57(4)
O(1)	0.3783(2)	0.7935(1)	0.0707(1)	3.3(1)
O(2)	0.5165(2)	0.8201(2)	0.1739(1)	3.5(1)
O(3)	0.3605(2)	0.9738(1)	0.0985(1)	3.6(1)
O(4)	-0.6166(2)	0.3955(2)	0.7379(1)	4.0(1)
O(5)	0.4789(2)	0.2753(1)	0.1202(1)	4.2(1)
O(6)	0.4914(2)	0.4296(2)	0.1777(1)	3.9(1)
O(7)	0.3042(2)	0.4382(1)	0.0857(1)	3.5(1)
O(8)	-0.6678(3)	-0.0872(2)	0.7306(1)	4.3(1)
O(9)	1.0619(2)	0.5851(2)	0.0940(1)	3.9(1)
O(10)	0.8820(2)	0.4699(1)	0.0853(1)	3.8(1)
O(11W)	0.7561(3)	0.2951(2)	0.2387(1)	5.2(2)
N(1)	-0.1832(3)	0.6978(2)	0.4177(1)	3.7(2)
N(2)	-0.1812(3)	0.5932(2)	0.4451(1)	3.4(2)
N(3)	-0.1257(3)	0.1750(2)	0.4475(1)	3.6(2)
N(4)	-0.1634(2)	0.0759(2)	0.4603(1)	3.2(1)
N(5)	0.6416(3)	0.6264(2)	0.0660(1)	2.8(1)
N(6)	1.3534(3)	0.9180(2)	-0.1004(2)	3.0(2)
C(1)	0.1976(3)	0.8122(2)	0.2106(1)	2.5(2)
C(2)	0.1376(4)	0.8753(2)	0.2654(2)	3.7(2)
C(3)	0.0079(4)	0.8375(3)	0.3315(2)	4.3(2)
C(4)	-0.0583(3)	0.7349(2)	0.3441(2)	3.2(2)
C(5)	-0.0022(4)	0.6748(3)	0.2877(2)	3.8(2)
C(6)	0.1256(3)	0.7123(3)	0.2209(2)	3.6(2)

Positional parameters and B(eq) for HABS/DL-Lysine J2142-33

atom	x	y	z	B(eq)
C(7)	-0.3001(3)	0.5488(2)	0.5191(2)	3.0(2)
C(8)	-0.4329(3)	0.6085(2)	0.5528(2)	3.4(2)
C(9)	-0.5380(3)	0.5559(2)	0.6251(2)	3.6(2)
C(10)	-0.5109(3)	0.4436(2)	0.6652(2)	3.0(2)
C(11)	-0.3815(4)	0.3840(2)	0.6309(2)	3.5(2)
C(12)	-0.2762(3)	0.4358(2)	0.5579(2)	3.6(2)
C(13)	0.2385(3)	0.3068(2)	0.2376(2)	2.6(2)
C(14)	0.1790(3)	0.3646(2)	0.2958(2)	3.5(2)
C(15)	0.0590(4)	0.3185(3)	0.3641(2)	3.8(2)
C(16)	-0.0014(3)	0.2144(2)	0.3748(2)	2.9(2)
C(17)	0.0587(3)	0.1573(2)	0.3157(2)	3.2(2)
C(18)	0.1783(3)	0.2027(2)	0.2472(2)	3.0(2)
C(19)	-0.2903(3)	0.0372(2)	0.5313(2)	2.9(2)
C(20)	-0.3702(4)	0.1019(2)	0.5826(2)	3.8(2)
C(21)	-0.4954(4)	0.0590(3)	0.6480(2)	4.2(2)
C(22)	-0.5420(3)	-0.0498(2)	0.6644(2)	3.2(2)
C(23)	-0.4632(3)	-0.1155(2)	0.6144(2)	3.1(2)
C(24)	-0.3376(3)	-0.0717(2)	0.5481(2)	3.1(2)
C(25)	0.9196(3)	0.5611(2)	0.0830(1)	2.6(2)
C(26)	0.8062(3)	0.6641(2)	0.0668(2)	2.5(2)
C(27)	0.8656(3)	0.7539(2)	-0.0146(2)	3.0(2)
C(28)	1.0210(3)	0.8118(2)	-0.0172(2)	3.0(2)
C(29)	1.0523(3)	0.9140(2)	-0.0930(2)	3.3(2)
C(30)	1.1944(3)	0.9824(2)	-0.0967(2)	3.4(2)
H(2)	0.188(3)	0.942(2)	0.257(2)	4.5

J2142-34

Positional parameters and B(eq) for HABS/DL-Lysine

atom	x	y	z	B(eq)
H(3)	-0.035(4)	0.880(2)	0.370(2)	4.9
H(4O)	-0.576(4)	0.329(3)	0.753(2)	4.8
H(5)	-0.045(3)	0.611(2)	0.294(2)	4.6
H(5A)	0.652(3)	0.602(2)	0.022(2)	4.0
H(5B)	0.610(3)	0.560(2)	0.113(2)	4.0
H(5C)	0.572(3)	0.682(2)	0.067(2)	4.0
H(6)	0.167(3)	0.668(2)	0.182(2)	4.2
H(6A)	1.436(3)	0.960(2)	-0.105(2)	4.0
H(6B)	1.372(3)	0.890(2)	-0.142(2)	4.0
H(6C)	1.354(3)	0.859(2)	-0.058(2)	4.0
H(8O)	-0.691(4)	-0.149(3)	0.733(2)	5.1
H(8)	-0.451(3)	0.685(2)	0.523(2)	4.0
H(9)	-0.626(3)	0.598(2)	0.649(2)	4.3
H(9O)	1.127(3)	0.528(2)	0.097(2)	4.0
H(11)	-0.367(3)	0.310(2)	0.657(2)	4.2
H(11W)	0.842(4)	0.318(3)	0.206(2)	6.0
H(11A)	0.679(4)	0.344(3)	0.209(2)	6.0
H(12)	-0.183(3)	0.394(2)	0.531(2)	4.3
H(14)	0.225(3)	0.429(2)	0.291(2)	4.2
H(15)	0.015(3)	0.354(2)	0.406(2)	4.5
H(17)	0.018(3)	0.094(2)	0.325(2)	3.8
H(18)	0.222(3)	0.161(2)	0.204(2)	3.5
H(20)	-0.341(3)	0.177(2)	0.567(2)	4.5
H(21)	-0.546(4)	0.097(2)	0.682(2)	4.9
H(23)	-0.496(3)	-0.188(2)	0.624(2)	3.7

J214/2-35

Positional parameters and B(eq) for HABS/DL-Lysine

atom	x	y	z	B(eq)
H(24)	-0.280(3)	-0.114(2)	0.515(2)	3.7
H(26)	0.790(3)	0.694(2)	0.115(1)	3.1
H(27A)	0.885(3)	0.715(2)	-0.057(2)	3.5
H(27B)	0.774(3)	0.813(2)	-0.019(1)	3.5
H(28A)	1.121(3)	0.758(2)	-0.017(2)	3.6
H(28B)	1.017(3)	0.831(2)	0.034(2)	3.6
H(29A)	1.074(3)	0.891(2)	-0.145(2)	3.9
H(29B)	0.949(3)	0.961(2)	-0.094(2)	3.9
H(30A)	1.208(3)	1.052(2)	-0.147(2)	4.2
H(30B)	1.181(3)	1.006(2)	-0.051(2)	4.2

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U values for HABS/DL-Lysine

atom	U11	U22	U33	U12	U13	U23
S(1)	0.0319(3)	0.0336(4)	0.0314(3)	-0.0025(2)	-0.0045(3)	-0.0089(3)
S(2)	0.0297(3)	0.0314(3)	0.0362(4)	0.0015(2)	-0.0085(3)	-0.0086(3)
O(1)	0.047(1)	0.048(1)	0.033(1)	-0.0026(8)	-0.0044(8)	-0.0197(9)
O(2)	0.036(1)	0.053(1)	0.044(1)	-0.0025(8)	-0.0136(8)	-0.012(1)
O(3)	0.044(1)	0.030(1)	0.056(1)	-0.0026(8)	-0.001(1)	-0.0053(9)
O(4)	0.053(1)	0.054(1)	0.038(1)	-0.010(1)	0.006(1)	-0.008(1)
O(5)	0.047(1)	0.038(1)	0.065(1)	0.0128(9)	0.004(1)	-0.018(1)
O(6)	0.047(1)	0.059(1)	0.045(1)	-0.022(1)	-0.0117(9)	-0.013(1)
O(7)	0.045(1)	0.049(1)	0.034(1)	0.0123(8)	-0.0129(8)	-0.0052(9)
O(8)	0.061(1)	0.060(1)	0.041(1)	-0.017(1)	0.008(1)	-0.018(1)
O(9)	0.047(1)	0.042(1)	0.074(1)	0.0128(9)	-0.035(1)	-0.028(1)
O(10)	0.044(1)	0.033(1)	0.065(1)	-0.0007(8)	-0.007(1)	-0.013(1)
O(11W)	0.053(1)	0.063(2)	0.072(2)	-0.007(1)	-0.023(1)	0.006(1)
N(1)	0.047(1)	0.047(1)	0.041(1)	-0.008(1)	0.003(1)	-0.008(1)
N(2)	0.041(1)	0.053(2)	0.033(1)	-0.009(1)	-0.004(1)	-0.010(1)
N(3)	0.044(1)	0.049(1)	0.042(1)	-0.008(1)	-0.003(1)	-0.013(1)
N(4)	0.038(1)	0.044(1)	0.038(1)	-0.005(1)	-0.010(1)	-0.008(1)
N(5)	0.034(1)	0.036(1)	0.037(1)	-0.001(1)	-0.005(1)	-0.012(1)

U values for HABS/DL-Lysine

atom	U11	U22	U33	U12	U13	U23
N(6)	0.034(1)	0.038(1)	0.044(1)	-0.003(1)	-0.005(1)	-0.015(1)
C(1)	0.033(1)	0.035(1)	0.029(1)	-0.001(1)	-0.009(1)	-0.009(1)
C(2)	0.053(2)	0.034(2)	0.049(2)	-0.008(1)	0.007(1)	-0.014(1)
C(3)	0.063(2)	0.041(2)	0.049(2)	-0.005(1)	0.016(2)	-0.018(1)
C(4)	0.037(1)	0.046(2)	0.034(1)	-0.004(1)	-0.003(1)	-0.009(1)
C(5)	0.053(2)	0.056(2)	0.042(2)	-0.025(1)	-0.002(1)	-0.019(2)
C(6)	0.051(2)	0.056(2)	0.035(2)	-0.019(1)	-0.001(1)	-0.022(1)
C(7)	0.038(1)	0.049(2)	0.028(1)	-0.007(1)	-0.005(1)	-0.012(1)
C(8)	0.049(2)	0.041(2)	0.037(2)	-0.004(1)	-0.007(1)	-0.009(1)
C(9)	0.045(2)	0.047(2)	0.044(2)	-0.000(1)	0.000(1)	-0.017(1)
C(10)	0.040(1)	0.046(2)	0.029(1)	-0.009(1)	-0.006(1)	-0.012(1)
C(11)	0.053(2)	0.043(2)	0.034(2)	0.001(1)	-0.009(1)	-0.006(1)

C(12)	0.047(2)	0.049(2)	0.037(2)	0.004(1)	-0.001(1)	-0.012(1)
C(13)	0.030(1)	0.033(1)	0.034(1)	0.001(1)	-0.012(1)	-0.006(1)
C(14)	0.049(2)	0.038(2)	0.049(2)	-0.009(1)	-0.005(1)	-0.019(1)
C(15)	0.053(2)	0.048(2)	0.044(2)	-0.008(1)	0.002(1)	-0.022(1)
C(16)	0.039(1)	0.040(2)	0.033(1)	-0.003(1)	-0.008(1)	-0.009(1)
C(17)	0.044(1)	0.032(1)	0.045(2)	-0.009(1)	-0.010(1)	-0.007(1)

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U values for HABS/DL-Lysine

atom	U11	U22	U33	U12	U13	U23
C(18)	0.042(1)	0.035(2)	0.037(2)	-0.001(1)	-0.007(1)	-0.013(1)
C(19)	0.036(1)	0.045(2)	0.032(1)	-0.004(1)	-0.010(1)	-0.009(1)
C(20)	0.057(2)	0.043(2)	0.044(2)	-0.011(1)	-0.004(1)	-0.017(1)
C(21)	0.062(2)	0.054(2)	0.044(2)	-0.008(2)	0.004(1)	-0.025(2)
C(22)	0.043(1)	0.050(2)	0.027(1)	-0.007(1)	-0.005(1)	-0.010(1)
C(23)	0.044(1)	0.037(2)	0.035(1)	-0.004(1)	-0.011(1)	-0.007(1)
C(24)	0.039(1)	0.045(2)	0.034(2)	0.002(1)	-0.009(1)	-0.012(1)
C(25)	0.037(1)	0.034(2)	0.029(1)	0.003(1)	-0.006(1)	-0.013(1)
C(26)	0.031(1)	0.035(1)	0.033(1)	0.001(1)	-0.007(1)	-0.015(1)
C(27)	0.034(1)	0.037(2)	0.041(2)	0.000(1)	-0.009(1)	-0.010(1)
C(28)	0.036(1)	0.035(2)	0.044(2)	-0.001(1)	-0.010(1)	-0.011(1)
C(29)	0.031(1)	0.044(2)	0.044(2)	0.001(1)	-0.007(1)	-0.006(1)
C(30)	0.038(1)	0.036(2)	0.055(2)	0.003(1)	-0.003(1)	-0.015(1)
H(2)	0.0574					
H(3)	0.0626					
H(4O)	0.0611					
H(5)	0.0576					
H(5A)	0.0507					

U values for HABS/DL-Lysine

atom	U11	U22	U33	U12	U13	U23
H(5B)	0.0507					
H(5C)	0.0507					

H(6)	0.0536
H(6A)	0.0507
H(6B)	0.0507
H(6C)	0.0507
H(8O)	0.0643
H(8)	0.0507
H(9)	0.0546
H(9O)	0.0507
H(11)	0.0534
H(11W)	0.0762
H(11A)	0.0762
H(12)	0.0544
H(14)	0.0529
H(15)	0.0574
H(17)	0.0483
H(18)	0.0446

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U values for HABS/DL-Lysine

atom	U11	U22	U33	U12	U13	U23
H(20)	0.0572					
H(21)	0.0620					
H(23)	0.0466					
H(24)	0.0469					
H(26)	0.0387					
H(27A)	0.0448					
H(27B)	0.0448					
H(28A)	0.0458					
H(28B)	0.0458					
H(29A)	0.0497					
H(29B)	0.0497					
H(30A)	0.0527					
H(30B)	0.0527					

Intramolecular Distances

J2142-39

atom	atom	distance	atom	atom	distance
S(1)	O(1)	1.460(2)	N(5)	H(5C)	0.86(3)
S(1)	O(2)	1.455(2)	N(6)	C(30)	1.474(3)
S(1)	O(3)	1.443(2)	N(6)	H(6A)	0.88(3)
S(1)	C(1)	1.766(2)	N(6)	H(6B)	0.86(3)
S(2)	O(5)	1.442(2)	N(6)	H(6C)	0.87(3)
S(2)	O(6)	1.445(2)	C(1)	C(2)	1.382(4)
S(2)	O(7)	1.461(2)	C(1)	C(6)	1.385(4)
S(2)	C(13)	1.765(2)	C(2)	C(3)	1.383(4)
O(4)	C(10)	1.364(3)	C(2)	H(2)	0.93(3)
O(4)	H(4O)	0.85(3)	C(3)	C(4)	1.385(4)
O(8)	C(22)	1.362(3)	C(3)	H(3)	0.96(3)
O(8)	H(8O)	0.80(3)	C(4)	C(5)	1.371(4)
O(9)	C(25)	1.309(3)	C(5)	C(6)	1.378(4)
O(9)	H(9O)	0.85(3)	C(5)	H(5)	0.87(3)
O(10)	C(25)	1.199(3)	C(6)	H(6)	0.98(3)
O(11W)	H(11W)	0.82(3)	C(7)	C(8)	1.387(4)
O(11W)	H(11A)	0.96(3)	C(7)	C(12)	1.385(4)
N(1)	N(2)	1.252(3)	C(8)	C(9)	1.370(4)
N(1)	C(4)	1.432(3)	C(8)	H(8)	0.95(3)
N(2)	C(7)	1.424(3)	C(9)	C(10)	1.387(4)
N(3)	N(4)	1.252(3)	C(9)	H(9)	0.94(3)
N(3)	C(16)	1.424(3)	C(10)	C(11)	1.372(4)
N(4)	C(19)	1.418(3)	C(11)	C(12)	1.376(4)
N(5)	C(26)	1.490(3)	C(11)	H(11)	0.91(3)
N(5)	H(5A)	0.87(3)	C(12)	H(12)	1.00(3)
N(5)	H(5B)	0.98(3)	C(13)	C(14)	1.380(4)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances (cont)

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atom	atom	distance
C(13)	C(18)	1.392(3)
C(14)	C(15)	1.375(4)
C(14)	H(14)	0.89(3)
C(15)	C(16)	1.388(4)
C(15)	H(15)	0.94(3)
C(16)	C(17)	1.385(4)
C(17)	C(18)	1.372(4)
C(17)	H(17)	0.85(3)
C(18)	H(18)	1.00(3)
C(19)	C(20)	1.388(4)
C(19)	C(24)	1.385(4)
C(20)	C(21)	1.365(4)
C(20)	H(20)	0.94(3)
C(21)	C(22)	1.382(4)
C(21)	H(21)	0.87(3)
C(22)	C(23)	1.378(4)
C(23)	C(24)	1.378(3)
C(23)	H(23)	0.93(3)
C(24)	H(24)	0.91(3)
C(25)	C(26)	1.511(3)
C(26)	C(27)	1.522(3)
C(26)	H(26)	0.97(2)
C(27)	C(28)	1.524(4)
C(27)	H(27A)	0.96(3)
C(27)	H(27B)	1.01(3)
C(28)	C(29)	1.519(4)
C(28)	H(28A)	1.01(3)
C(28)	H(28B)	0.96(3)
C(29)	C(30)	1.502(4)
C(29)	H(29A)	0.98(3)
C(29)	H(29B)	0.99(3)
C(30)	H(30A)	1.02(3)
C(30)	H(30B)	0.90(3)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.